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Physics Procedia 2 (2009) 839–844

Physics Procedia

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Proceedings of the JMSM 2008 Conference

Contribution to the study of recombination at the interface spherical precipitate / p-type semiconductor in the EBIC mode.

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Received 1 January 2009; received in revised form 31 July 2009; accepted 31 August 2009

Abstract

This work is a contribution to the understanding of some recombination processes occurring at the interface spherical precipitate/p-type semiconductor in the EBIC mode.

The calculations, which adopt a self consistent procedure and are in live with the Hall Shockley Read (SRH) framework, consist to appreciate the respective variations of the precipitate barrier height, E_b, and of the effective recombination velocity, S_{eff}, as a function of some physical parameters such as the precipitate size, R, the Read sphere, Ř, the interface state density, N_t, or the doping concentration, N_a.

The bending evolution of the minority carrier quasi Fermi level in the precipitate space charge and quasi neutral regions, Δ_1 and Δ_2 respectively, is taken into account, while the majority carrier one is considered constant.

The obtained results show in particular that S_{eff} and E_b strongly depend of the doping concentration, N_a, and of the interfacial state density of defects, N_t.

Moreover, it appears that S_{eff} is nearly proportional to $\exp(E_b / k_b T)$, in our operating conditions.

PACS: Type pacs here, separated by semicolons ;

Keywords: EBIC, recombination, p-type semiconductor, precipitate, self consistent calculation, SRH theory;

1. Introduction

It is now admitted that the presence of defects in semiconductors reduce their performances [1-2]. They effectively take place into electron-hole recombination processes by reducing their lifetime, leading to a significant modification of their properties, especially electronic and optical ones [3].

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doi:10.1016/j.phpro.2009.11.033

Many approaches have been proposed for the evolution understanding of some physical parameters characterizing the recombination at dislocations [4], grain boundaries [5], general defects [6] or punctuals [7], as well as precipitates [8].

The purpose of this contribution is to elaborate a theoretical model based on a self consistent procedure, which enables the behavior determination of the precipitate effective recombination velocity, S_{eff}, and of the barrier height, E_b, according to the density of interface states, N_t, the doping concentration, N_a, and the size, R.

The calculations are made into the SRH theory framework, assuming a monoenergetic distribution of the interface states in a Half Filled Level model [9].

2. Bases of the model

Figure 1 represents the variation of the energy bands and the quasi Fermi levels as a function of the distance at the spherical precipitate/p type semiconductor interface, under illuminated conditions.

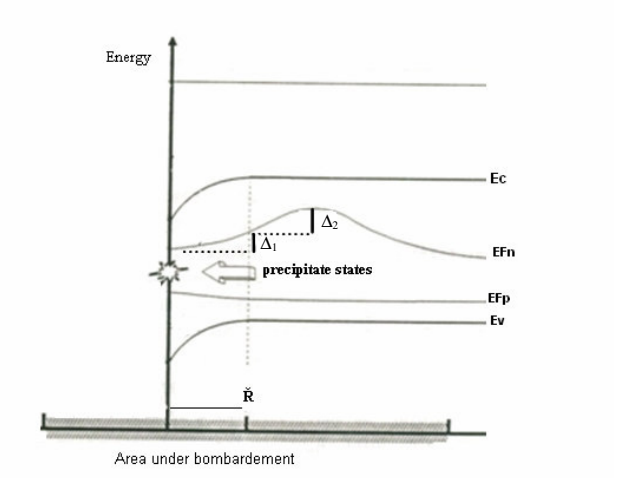

Fig. 1. Representative band diagram at the interface between a metallic precipitate and a p type semiconductor matrix.

The quasi Fermi level of the majority carriers, E_{Fp}, is assumed to be flat everywhere, but the minority carriers one, E_{Fn}, is allowed to vary in both space charge and quasi neutral regions, with bendings indicated by Δ_1 and Δ_2, respectively.

Moreover, the charge on the defect states, whose the energy level, E_t, is assumed to be located in the middle of the gap, is calculated on the basis of the Half-Filled-Level-Model (HFLM) by the following equation:

$$Q = eN_t \left| \frac{1}{2} - f \right| 4\pi R^2 \tag{1}$$

where Nt stands for the defect number per unit area, e the elementary charge, R, the precipitate size and f the defect occupation probability.

Q compensates another charge Q' derived from the doping ionization process, in a region located between R and Ř, this latter being the Read sphere.

Q' can be expressed as:

$$Q' = Q = \frac{4}{3}\pi eNa(\tilde{R}^3 - R^3) \tag{2}$$

where Na is the doping concentration.

Therefore, from the Poisson equation, it is easy to establish an expression for the barrier height, Eb, at the bottom of the space charge region, i.e., at Ř-R.

All calculations made, we obtain:

$$E_b = \frac{e^2 Na}{2\varepsilon}\tilde{R}^2 - \frac{e^2 Na}{3\varepsilon}\left[\frac{\tilde{R}^3}{R} + \frac{R^2}{2}\right] \quad (3)$$

ε represents the dielectric constant of the semiconductor.

Indeed, the occupation probability f of the defect levels is governed by the SRH formalism and depends on the energy level Et, as well as the hole and electron concentrations on the precipitate surface, n(R) and p(R) respectively. Its expression is:

$$f = \frac{n(R) + n_i \exp\left[(E_i - E_t)/k_b T\right]}{n(R) + p(R) + 2n_i \cosh\left[(E_t - E_i)/k_b T\right)]} \quad (4)$$

ni is the intrinsic carrier concentration, T the absolute temperature and k_b the Boltzmann constant.

With the assumption of a flat majority carrier quasi-Fermi level, p(R) and n (R) are given by:

$$p(R) = \frac{N_a + \sqrt{N_a^2 + 4\,n_i^2}}{2} \exp\left[-\frac{E_b}{k_b T}\right] \quad (5)$$

$$n(R) = \frac{n_i^2}{p_o} \exp\left[\frac{\Delta(R) + E_b}{k_b T}\right] \quad (6)$$

Where p_o is the hole concentration, at equilibrium.

$\Delta(R) = E_{Fn}(R) - E_{Fp}$ represents the excitation level at the interface. It is related to the excitation Δ, which is equal to $\Delta = [E_{Fn}(\infty) - E_{Fp}]$, by the following relation:

$$\Delta = [E_{Fn}(\infty) - E_{Fn}(\check{R})] + [E_{Fn}(\check{R}) - E_{Fn}(R)] + [E_{Fn}(R) - E_{Fp}] \quad (7)$$

Let us introduce the bendings Δ_1 and Δ_2 as:

$$\Delta_1 = \left|E_{F_n}(\tilde{R}) - E_{F_n}(R)\right| \quad \text{and} \quad \Delta_2 = \left|E_{F_n}(\infty) - E_{F_n}(\tilde{R})\right| \quad (8)$$

It follows that equation (7) becomes:

$$\Delta = \Delta_2 + \Delta_1 + \Delta(R) \quad (9)$$

Furthermore, the net recombination rate at the interface, Us, is determined by the well-known SRH expression:

$$U_s = \sigma V_{th} N_t \frac{n(R)\,p(R) - n_i^2}{n(R) + p(R) + 2n_i \cosh\left[(E_i - E_t)/k_b T\right)]} \quad (10)$$

Where V_{th} is the thermal velocity and σ the capture cross section assumed the same for electron and holes.

In the absence of generation and recombination of carriers in the space charge region, the minority flow, $J_n(r)$, can be connected to U_s as follows:

$$-U_s = 4\pi r^2 J_n(r) = e\,D_n\,n(r)\left(\frac{\partial}{\partial r} E_{F_n}(r)\right) \quad (11)$$

Where n(R) equals:

$$n(r) = n_i \exp\left[\frac{E_{Fn}(r) - E_i(r)}{k_b T}\right] \quad (12)$$

D_n is the electron diffusion coefficient.

Combining relations (3),(6),(10 -11) and after solving first the diffusion equation in the depletion zone and second the spatial dependence of the minority carrier quasi Fermi level, it is found that the electron concentration at the interface, on the Read sphere, is such that :

$$n(\tilde{R}) = n(R) \exp\left(-\frac{E_b}{k_b T}\right) + U_S F_0 \quad (13)$$

With

$$F_0 = \exp\left\{\frac{E_i(\tilde{R}) - E_b - \frac{e^2 Na}{3\varepsilon}\left(\frac{\tilde{R}^3}{R} + \frac{R^2}{2}\right)}{k_b T}\right\} \int_{R}^{\tilde{R}} \frac{\exp\left(\frac{e^2 Na}{3\varepsilon}\left[\frac{\tilde{R}^3}{r} + \frac{r^2}{2}\right]\right)}{r^2} dr \quad (14)$$

An effective recombination velocity, S_{eff}, can be defined as:

$$S_{eff} = \frac{U_S}{4\pi\tilde{R}^2\left[n(\tilde{R}) - n_o\right]} \quad (15)$$

Finally, taking into account n(R) at R, $\breve{R}$ and infinite positions allows expressions of Δ_1 and Δ_2 as:

$$\Delta_1 = E_{Fn}(\tilde{R}) - E_{Fn}(R) = E_b + k_b T \ln\left(\frac{n(\tilde{R})}{n(R)}\right) \quad (16)$$

and

$$\Delta_2 = k_b T \ln\left(\frac{n(\infty)}{n(\tilde{R})}\right) = k_b T \ln\left(1 - \frac{\tilde{R} S_{eff}}{D_n\left(\frac{\tilde{R}}{L_n} + 1\right)}\right)\left(1 - \frac{n_0}{n(\tilde{R})}\right) \quad (17)$$

From relations (16) and (17), it clearly appears that the knowledge of Δ_1 and Δ_2 permitts the determination of E_b and S_{eff}, under the self consistent approach discussed above.

3. Results and discussion

Figures (2.a) and (2.b) characterize the variation of Δ_1 and Δ_2 as a function of the bulk excitation level E_{Fn}-E_{Fp} = Δ, for two size precipitates, infinite and 1500 (Å), respectively.

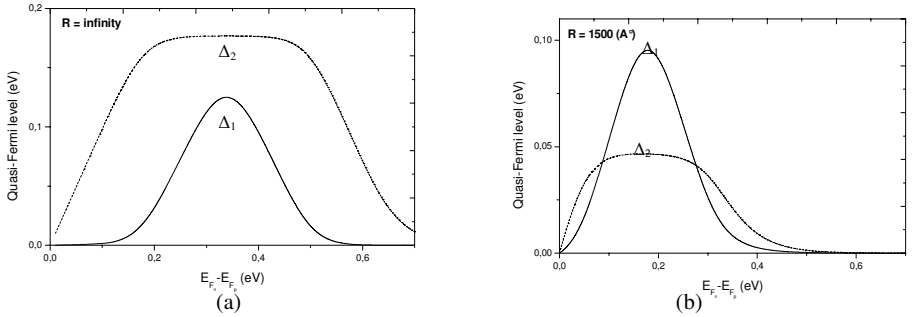

Fig. 2. Bendings of the minority carrier quasi -Fermi level in the precipitate space charge region (Δ_1) and in the quasi-neutral region (Δ_2) vs the bulk excitation level (Δ), for two precipitate sizes.

a : R=∞, b : R=1500 (A°).

σ=2.10^{-16} (cm^{-2}), L_n=50 (μm), D_n=14 (cm^2/s) and N_a=10^{16} (cm^{-3}), N_t=8.10^{11} (cm^{-2}).

The general shape of these curves shows a symmetric behaviour around an identical Δ value, this latter being higher for large precipitate size.

Moreover, Δ_1 and Δ_2 equal zero at very low and very high excitation; nevertheless, these results agree with different physical explications:

At low excitation, the flow of minority excess charge carriers is low, the quasi Fermi levels are then not affected, whereas at high excitation, the excess charge carriers tend to saturate the interface states associated with the precipitate.

The junction point is the Δ_1 and Δ_2 curve maximum; from this particular point, it appears in fact that the effective recombination velocity, S_{eff}, decreases.

Figures (3.a) and (3.b) confirm this assertion.

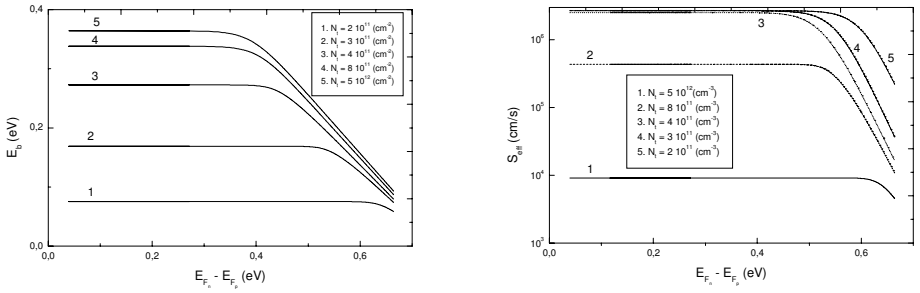

Fig. 3. Evolution of the interface barrier height, E_b, and the effective recombination velocity, S_{eff}, with the excitation level, Δ, for different interface defect state densities, N_t.
R = infinity, $N_a = 10^{16}$ (cm^{-3}), L_n= 50 (μm), D_n = 14 (cm^2/s), T = 300 (K°).
1. $N_t = 5\ 10^{12}$ (cm^{-2}), 2. $N_t = 8\ 10^{11}$ (cm^{-2}), 3. $N_t = 4\ 10^{11}$ (cm^{-2}), 4. $N_t = 3\ 10^{11}$ (cm^{-2}), 5. $N_t = 10^{11}$ (cm^{-2}).

At low excitation ($E_{Fn} - E_{Fp} \approx 0$), i.e., near the precipitate, a quite important charge quantity can exist, large enough to cause a significant recombination.

When the excitation increases, i.e., when moving more and more of the precipitate, the excess minority carriers gradually fill the interface states up to saturation, causing the decrease of E_b and thus of S_{eff}.

The doping effect on S_{eff} has been also studied, it is reported in Figure 4.

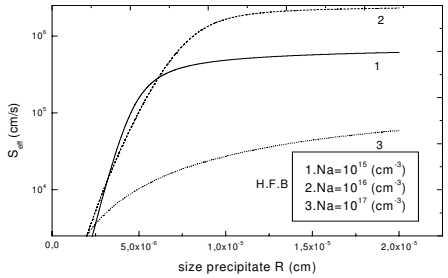

Fig. 4. Evolution of the effective recombination velocity, S_{eff}, according to the precipitate size, R, for various doping concentration, N_a:
Nt = 8 10^{11} (cm^2), σ = 2 10^{-15} (cm^2), L = 80 (μm); D_n = f (N_a) [10], T = 300 (K°).
1. $N_a = 10^{15}$ (cm^3), 2. $N_a = 10^{16}$ (cm^3), 3. $N_a = 10^{17}$ (cm^3).

The variation of these curves can be explained, again, by the gradual filling of trap centers for the bottom of graphs and a saturation effect of these centers for the constant part of graphs.

Concerning the doping influence, it appears that S_{eff} is even higher than N_a is important, mainly due to charge quantity available and this, until a critical value of N_a equal to 10^{17} cm^{-3}, confirming some results of literature [5].

From that point, the occupation function, f, decreases sharply.

The analysis of this situation is not obvious, just not that the decrease of the precipitate electrical activity is not always directly related to the doping concentration growth.

Phenomena such as segregation or doping ionization can also play a role.

The respective influences of the two main recombination parameters, namely E_b and S_{eff}, are shown in Figure (5).

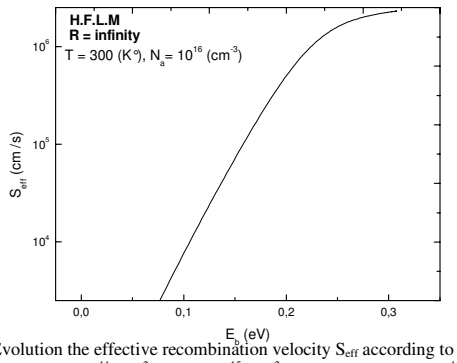

Fig. 5. Evolution the effective recombination velocity S_{eff} according to the barrier height, E_b.
R= infunity, $N_t = 8\ 10^{11}$ (cm^2), $\sigma = 2\ 10^{-15}$ (cm^2), L = 50 (µm), $N_a = 10^{16}$ (cm^3), T = 300 (K°).

The shape of this curve is qualitatively similar to those found in the literature [5]; in addition, an exponential form of S_{eff} evolution as a function of E_b have been found , confirming some older work results [5, 9].

4. Conclusion

The behaviour of two characteristic physical parameters of the recombination process at the interface spherical precipitate /p-type semiconductor, in the EBIC mode, namely the barrier height, E_b, and the effective recombination velocity, S_{eff}, has been investigated in the framework of a self consistent approach, using the Shockley Read Hall (SRH) theory for the charge carrier generation-recombination phenomena.

The main results obtained can be summarized as follows:

-The S_{eff} and E_b variation depend on the doping level, N_a, and on the state interface density, N_t.

-The quasi-Fermi level of the minority charge carriers have been derived, determined and taken into account in calculations.

-The dependence law of S_{eff} as a function of E_b admits an exponential form.

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